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Opacity: A window into High Energy Density Plasma Physics

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Overview

Opacity is a fundamental property of matter and knowledge of it is required to understand the transport of radiation through a material. Exact knowledge of opacity is crucial in many fields such as astrophysics, which recently produced a white paper on the current state of astrophysical opacities [1], plasma physics, including inertial confinement fusion (ICF) and magnetic confinement fusion, high energy density physics (HEDP), the semiconductor industry [2] and stockpile stewardship. In industry, the accurate knowledge of the opacity of tin is important for extreme ultraviolet (EUV) lithography and the development of processors with smaller components. In astrophysics, Cepheid variable stars are used as “standard candles” for determining the distance to objects. Opacities of these stars are required to understand the relationship between their periodicity, luminosity and distance. Our sun is the most studied star and provides the basis of our understanding for other stars. Yet in significant ways the sun is poorly understood. In recent years, there has been a debate over the abundances of heavy elements ($Z > 2$) in the solar interior. Current solar atmosphere models [3] find a significantly lower abundance for C, N, and O compared to models used roughly a decade ago. Although solar evolution models have matured, a discrepancy still exists between spectroscopic solar models (which require opacities) with updated abundances, and solar properties inferred from helioseismology and neutrinos [4]. Despite its necessity, opacity is not solved, and is an open and active area of research needed for improving our understanding of plasma physics.

Theory

Opacity calculations require three ingredients rooted in initial atomic structure calculations [5]. The first is a model called an equation of state (EOS) that predicts the population of atomic / ionic energy levels for a given plasma temperature and density. The second ingredient is line strengths (for bound-bound transitions) and photoionization cross sections (for bound-free transitions), which are obtained from atomic wavefunctions. Scattering and free-free absorption must also be included (but will be less important in HEDP regimes). The third ingredient is a model that predicts the line shapes of bound-bound transitions and includes line broadening due to plasma electric microfields, to which the photon-absorbing ion is exposed. This line broadening is important because it can significantly fill in valleys between otherwise sharp bound-bound features. This affects the important harmonic mean of the opacity (the Rosseland mean). The devil is in the details of these three main ingredients, and a good opacity calculation must treat all three carefully.

The equation-of-state (EOS) model often starts with a thermodynamic consideration of the plasma. This may be in a chemical or physical picture [6]. Within plasmas in local thermodynamic equilibrium (LTE) the Saha-Boltzmann equation predicts the population of ionic species when given a set of energy levels (or configurations) for each relevant ion. This does not normally include effects of plasma density, which are important in HEDP.

While classical plasma physics models can adequately describe fully ionized plasmas, most opacities of interest arise from partially ionized plasmas. Such systems require a treatment of the electron-ion interactions, the internal energy of the ions, and the contributions from the free electrons. Ideally, such a description would also smoothly treat the effects of increasing plasma density. The Mihalas-Hummer-Dappen (MHD) EOS model is commonly used [7] and is implemented in the widely used OP opacity tables [8]. A more recent EOS model (known as ChemEOS) [6, 9], that uses the chemical picture starts from this MHD model but includes a number of additions and modifications. ChemEOS is used in the recently released LANL opacity tables [9, 10]. We also refer to the OPAL [11] and the legacy LEDCOP [12] tables.

The atomic physics data [13] that are needed for the EOS and for computing the atomic transition probabilities that make up the photoexcitation (bound-bound) contributions often come from an atomic structure code that assumes all ions are isolated (i.e. does not include plasma perturbations on the atomic wavefunctions). The atomic data may be within a configuration-averaged picture or where the atomic configurations are further split into their terms or levels. This term- or level-splitting usually comes with a significant additional computation cost, especially when the number of interacting levels exceed 10^6. Atomic structure may need to be semi- or fully relativistic for accuracy, and transitions beyond dipole-allowed may need to be included. Photoionization cross sections (making up the bound-free opacity contribution) are often computed in a perturbative manner (through the distorted-wave approximation) or in a close-coupling approach (often using R-matrix theory). The latter can be important for neutral and low-charged ions, but are usually not required for more highly-charged ions that exist at higher plasma temperatures.

At many conditions of interest line broadening can be dominated by collisions between free electrons and sometimes ions. Plasma microfields can significantly influence such broadening. Collisional line broadening models such as those by Lee [14], Baranger [15], and Dimitrijevic [16] vary in implementation in opacity models and can also considerably add to the computational cost of the opacity calculations. So far, most large-scale opacity efforts have been forced to use severe approximations for line-broadening models, due to the computational cost of accurate line shape determination for the large numbers (often > billions) of lines that need to be considered in comprehensive opacity tables. In many cases Voigt line profiles are assumed [17]. Much work is underway to come up with a computationally efficient, yet accurate, scheme for evaluating line shapes for opacities (eg the recent line shapes workshops [18]).

Sustained efforts to compute opacities for elements of interest and wide ranges of temperatures and densities have been underway for many years. Commonly used opacity tables have been produced by LLNL (the OPAL tables) [11], LANL (LEDCOP) [12] and a UK-led collaboration (the OP tables) [8]. More recently, LANL has produced a new generation of opacity tables (from the ATOMIC code [10, 19]), and other tables have been reported from France (using the OPAS and SCO-RCG codes) and from Israel.

Experiment

Opacity experiments are challenging to perform because they require precise understanding of the laboratory drive and equation of state in addition to high precision spectroscopy and control over experimental conditions. Opacities in plasmas residing in (LTE) differ from those that are outside of equilibrium (NLTE) making these separate research areas. Independent measurements of the plasma temperature and density that do not rely on the spectrum of the element in question are the ideal but again difficult to achieve. In many cases the theoretical models are underpinned by measurements of atomic data such as line broadening widths or oscillator strengths that were measured in very different regimes from those in which the models are now being applied for astrophysics, ICF, and HED.

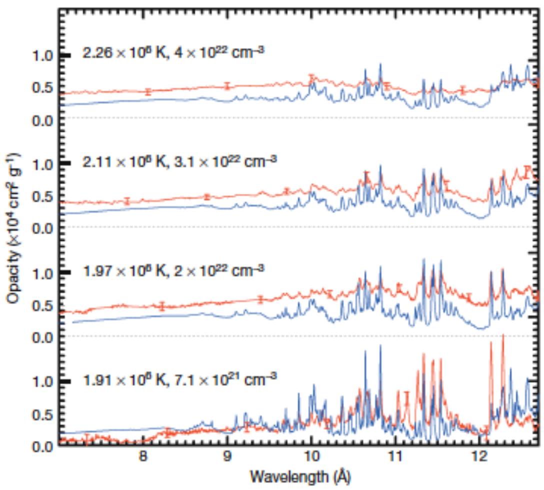

Figure 1 [21]: Compares Opacity-on-Z data (red) with SCRAM calculations (blue). Experiment and model differ significantly for the same conditions.

Near-LTE opacity experiments in the HED regime began in the 1990s and 2000s on high power systems of the day such as NOVA and short-pulse systems such as AWE's Helen laser [20, 21]. Since the last survey [22] experiments have been performed by LLNL to study Silicon opacity [23], in which discrepancies still exist between models and data for high-n transitions. On Sandia's Z-machine Bailey, et al [24] have measured iron opacity at temperatures and densities relevant to the solar radiation/convection zone boundary. Since the last survey [22], repeated scrutiny of the experiment and models has not produced a reason for the discrepancy shown in (Fig. 1). Experiments are underway on the NIF to attempt to recreate these results [25-27]. However, a resolution to this puzzle has not yet emerged. These discrepancies between model and experiment [24-28] pose a major challenge for our community. Research seeking solutions and studying opacities for other regimes or physical systems along this vein should be high priority.

The Opacity-on-NIF campaign is a 5-lab collaboration (LANL, LLNL, SNL, NNSS, LLE) currently dedicated to addressing this discrepancy by reproducing this measurement on a different platform. The first iron transmission at lower temperature (where Opacity-on-Z iron opacities agree with theory) has been completed [26]. Measurements at higher temperatures (where the disagreement between experiment and theory resides) are underway. Theoretical work is also underway to examine the applicability of the models to this question [29, 30].

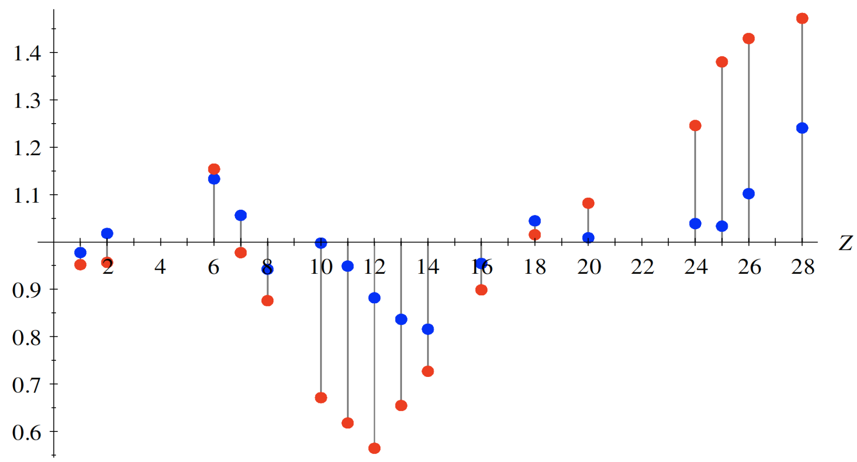

Figure 2: [26]. The red dots represent the ratio of the OPAS to the OP Rosseland mean opacity at T = 192 .91 eV and $N_e = 10^{23}$ cm^{-3}. Differences of up to 40% exist between the two models.

Within the same code, differences in the calculated opacity of up to 30% can occur depending on the model used. [27]. Even when comparing opacity codes that implement similar physics models, differences of up to 40% can exist, underscoring that the details of how calculations are performed are important [31-33] (Fig. 2). Physics differences may also exist between codes.

While a number of opacity experiments have been performed, these experiments sample a small range of the density and temperature phase space of interest. This provides a small span of conditions to benchmark models with experiment. In addition, many of these experiments were designed to measure the opacity and not necessarily test the model assumptions that go into the calculations.

Future Work and Areas for Investment

Looking ahead, there is need and opportunity for not only opacity values for multiple elements but specific pieces of atomic physics needed to benchmark opacity models in the HED regime. In addition to experiments currently being performed, additional platforms beyond that on Sandia's Z-machine and NIF should be encouraged. Close collaboration between modelers and experimentalists should provide guidance on future experiments to reduce uncertainty in assumptions in the models. For example, studying line shapes and cross sections at high spectral precision both in conditions we believe models predict correctly and in more challenging conditions. Experiments to improve our knowledge of EOS for opacities would also be valuable. Likewise, experiments on 'simpler' elements can be valuable for testing model assumptions at a particular set of conditions, because more complex electronic configurations may be included with less computational cost. One could also design experiments to help test whether thick tampers lead to non-uniform heating for opacity samples [34].

A greater emphasis on high resolution (1000 E/dE) x-ray spectroscopy on HED platforms is needed to conduct these experiments. Additionally, the ability to observe spectra in the soft x-ray regime (<1 keV) is currently limited by backgrounds and debris limits. Experiments at lower temperature and density conditions or with simpler targets that could be fielded on NIF or other facilities could help resolve this issue. Both opacity experiments on Sandia's Z machine and on NIF have had to design their own spectrometers to deal with these problems, which means the resources and capability to do so becomes a barrier to anyone attempting a high-resolution opacity or atomic physics measurement on these facilities. Encouraging measurements on a wide variety of facilities, such as new work on the LCLS XFEL [35] is also valuable for optimizing the ability of opacity measurements to reach a wide variety of relevant conditions. Additional effort spent on detection media would be highly valuable for enabling precise measurements. Current x-ray films are either legacy (and dwindling) or not calibrated, and electronic recording media do not yet achieve the same resolution as the best x-ray films.

In short, there is a great deal of work that should be performed in order to improve our understanding of the discrepancies between the different opacity models and between the opacity models and experiments. Knowledge of opacity is critical in many areas of research. With facilities such as the NIF and Sandia's Z-machine currently available to reach density and temperature conditions never obtained before, now is the time to extend our theoretical and experimental research programs to resolve the discrepancies.

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